Gradient Descent

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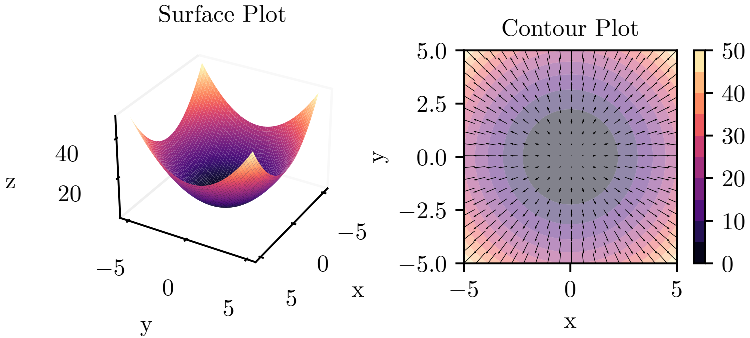
Contour Plot And Gradients

$$z = f(x, y) = x^2 + y^2$$



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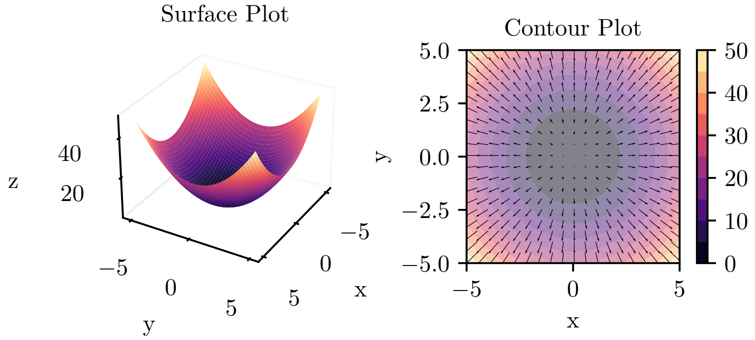

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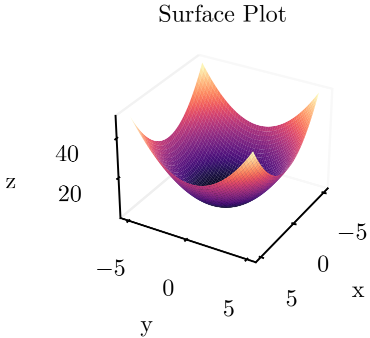

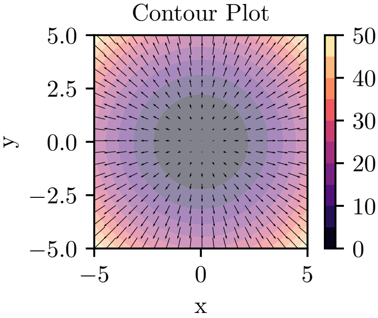

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$$\nabla f(x, y) = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

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- Note, here θ is the parameter vector

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- Goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \boldsymbol{f}(\boldsymbol{\theta}) \tag{2}$$

Introduction

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- It is an iterative algorithm
- It is a first order optimization algorithm
- It is a local search algorithm/greedy

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- where $\nabla^2 f(\mathbf{x}_0)$ is the Hessian matrix and $\nabla f(\mathbf{x}_0)$ is the gradient vector

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- We can write the second order Taylor's series as:
- $f(x) = 1 + 0(x - 0) + \frac{-1}{2!}(x - 0)^2 = 1 - \frac{x^2}{2}$

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- First order Taylor's series approximation is given by:
- $f(x) = f(x_0) + f'(x_0)(x - x_0) = 6 + 4(x - 2) = 4x - 2$

Taylor's Series (Alternative form)

- We have:

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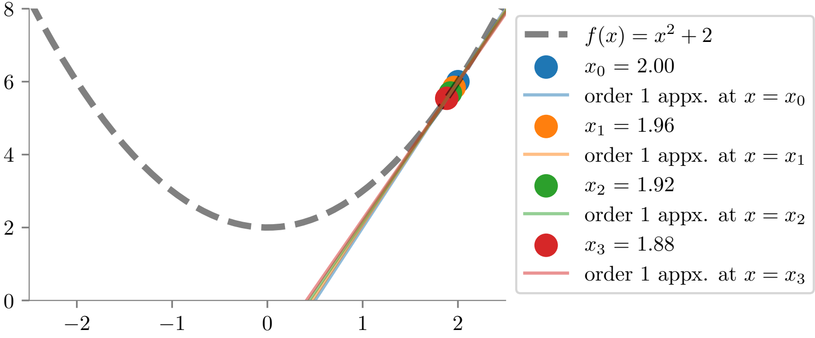
- This is the gradient descent algorithm: $\mathbf{x}_1 = \mathbf{x}_0 - \alpha \nabla f(\mathbf{x}_0)$

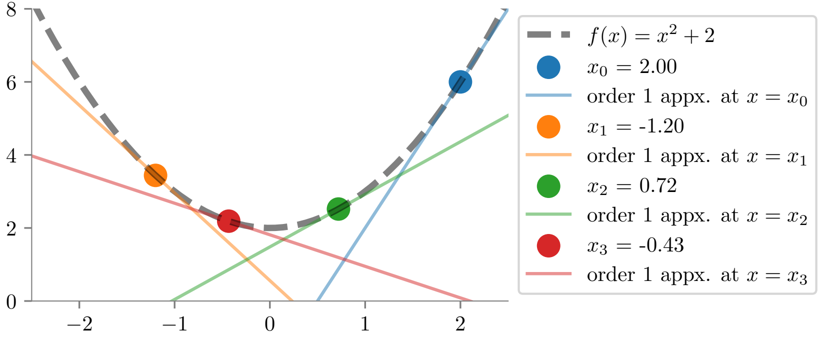
Effect of learning rate

Low learning rate $\alpha = 0.01$: Converges slowly



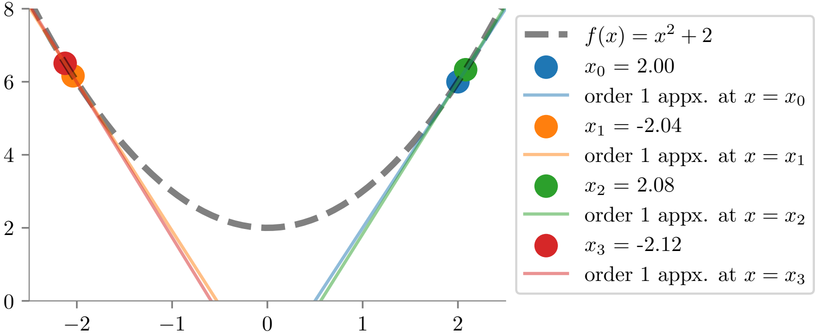
Effect of learning rate

High learning rate $\alpha = 0.8$: Converges quickly, but might overshoot



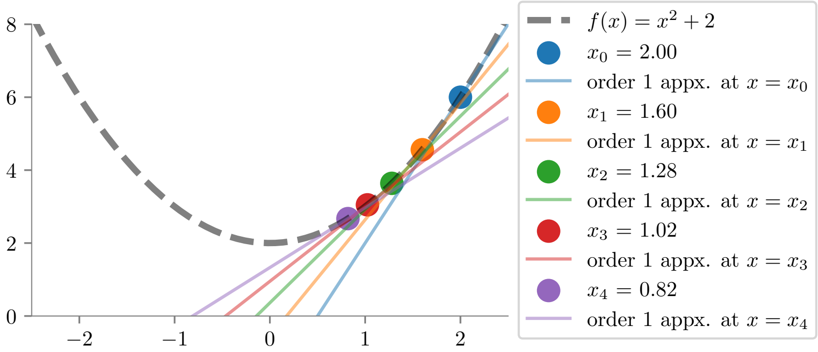
Effect of learning rate

Very high learning rate $\alpha = 1.01$: Diverges



Effect of learning rate

Appropriate learning rate $\alpha = 0.1$



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- **Objective function** is the most general term for any function that you optimize during training.

Gradient Descent : Example

Learn $y = \theta_0 + \theta_1 x$ on following dataset, using gradient descent where initially $(\theta_0, \theta_1) = (4, 0)$ and step-size, $\alpha = 0.1$, for 2 iterations.

x	y
1	1
2	2
3	3

Gradient Descent : Example

Our predictor, $\hat{y} = \theta_0 + \theta_1 x$

Error for i^{th} datapoint, $\epsilon_i = y_i - \hat{y}_i$
$\epsilon_1 = 1 - \theta_0 - \theta_1$
$\epsilon_2 = 2 - \theta_0 - 2\theta_1$
$\epsilon_3 = 3 - \theta_0 - 3\theta_1$

MSE = $\frac{\epsilon_1^2+\epsilon_2^2+\epsilon_3^2}{3}$ = $\frac{14+3\theta_0^2+14\theta_1^2-12\theta_0-28\theta_1+12\theta_0\theta_1}{3}$

Difference between SSE and MSE

$\sum \epsilon_i^2$ *increases as the number of examples increase*

So, we use MSE

$$MSE = \frac{1}{n} \sum \epsilon_i^2$$

Here n denotes the number of samples

Gradient Descent : Example

$$\frac{\partial \, \mathrm{MSE}}{\partial \theta_0} = \frac{2\sum_{i=1}^{n}(y_i - \theta_0 - \theta_1 x_i)(-1)}{n} = \frac{2\sum_{i=1}^{n}\epsilon_i(-1)}{n}$$

$$\frac{\partial \, \mathrm{MSE}}{\partial \theta_1} = \frac{2\sum_{i=1}^{n}(y_i - \theta_0 - \theta_1 x_i)(-x_i)}{n} = \frac{2\sum_{i=1}^{n}\epsilon_i(-x_i)}{n}$$

Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 4 - 0.2 \frac{((1-(4+0))(-1)+(2-(4+0))(-1)+(3-(4+0))(-1))}{3}$$

$$\theta_0 = 3.6$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Gradient Descent : Example

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$$\theta_1 = 0 - 0.2\frac{((1-(4+0))(-1)+(2-(4+0))(-2)+(3-(4+0))(-3))}{3}$$

$$\theta_1 = -0.67$$

Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.6 - 0.2 \frac{((1-(3.6-0.67))(-1)+(2-(3.6-0.67\times2))(-1)+(3-(3.6-0.67\times3))(-1))}{3}$$

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Gradient Descent : Example

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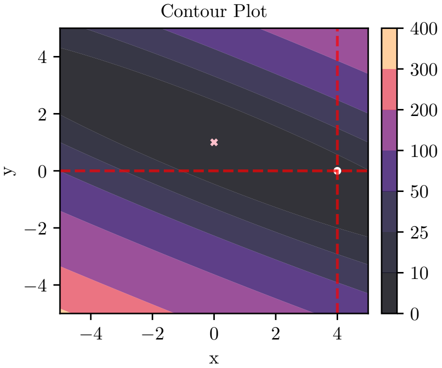
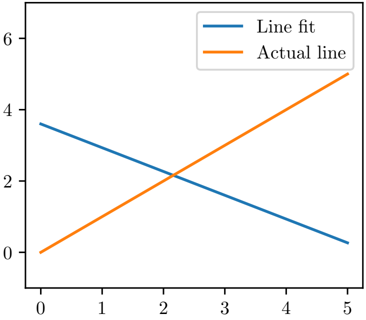
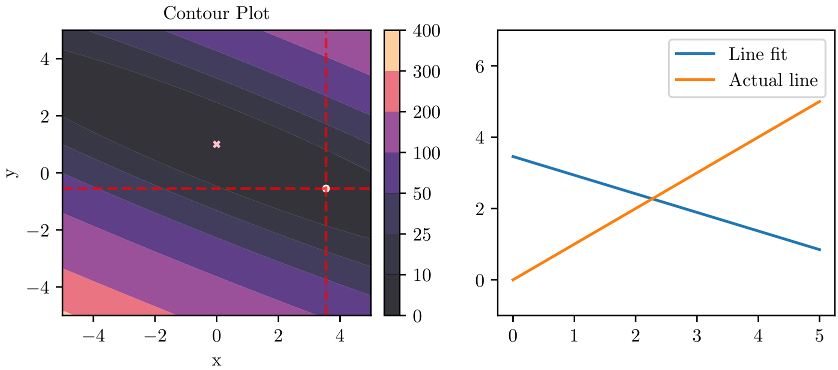
$$\theta_0 = -0.55$$

Gradient Descent : Example (Iteraion 0)

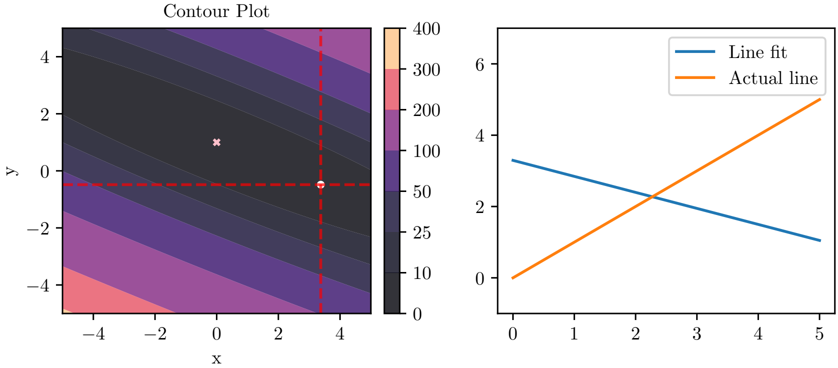




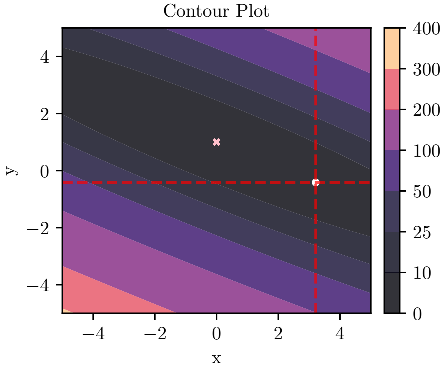
Gradient Descent : Example (Iteraion 2)

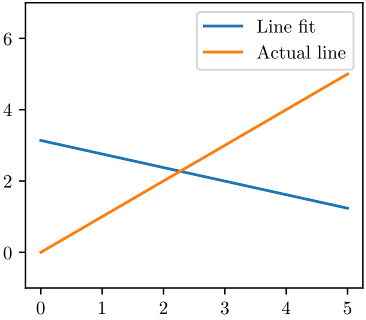


Gradient Descent : Example (Iteraion 4)

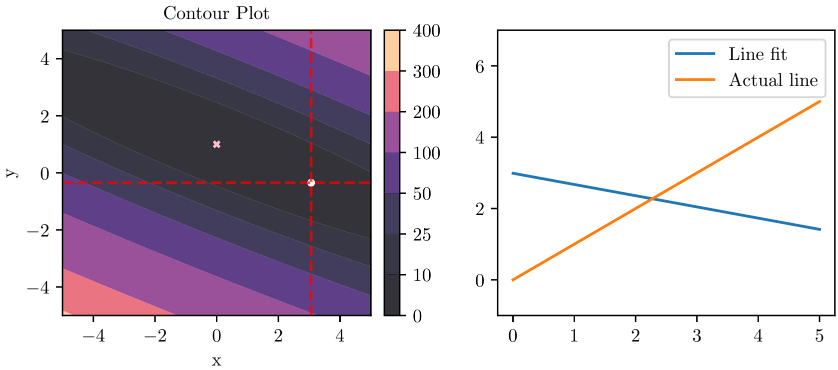


Gradient Descent : Example (Iteraion 6)

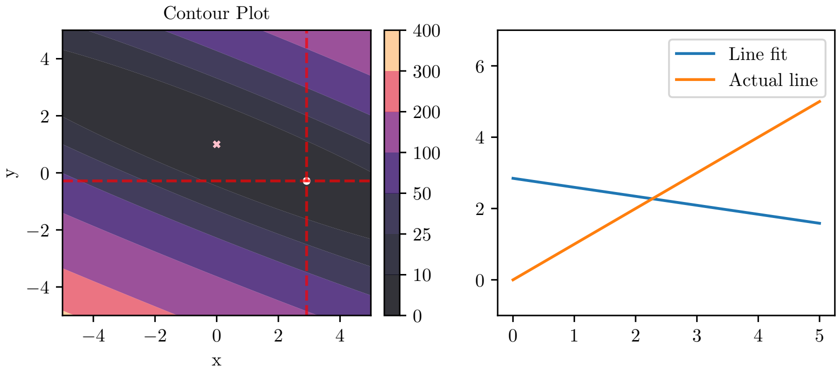




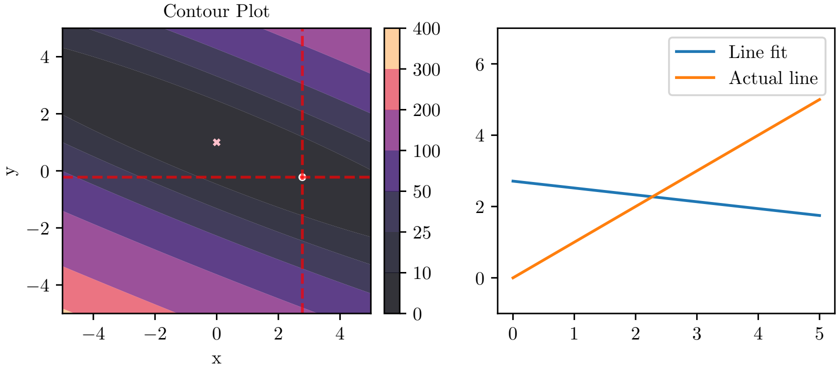
Gradient Descent : Example (Iteraion 8)



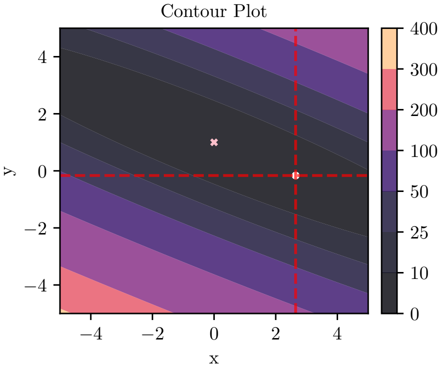
Gradient Descent : Example (Iteraion 10)

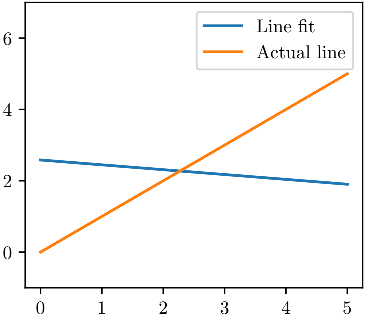


Gradient Descent : Example (Iteraion 12)

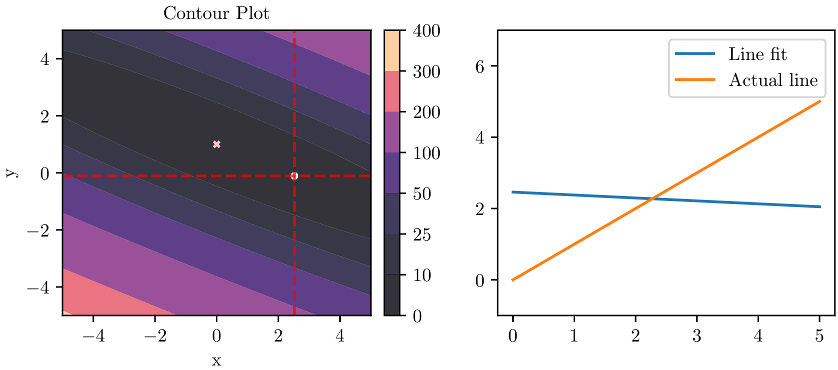


Gradient Descent : Example (Iteraion 14)

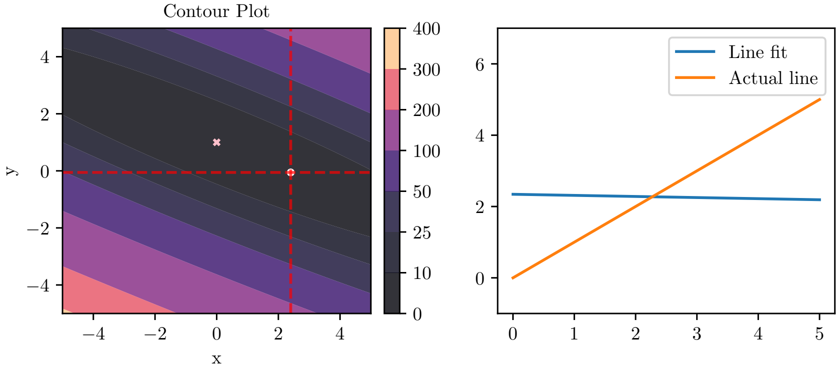




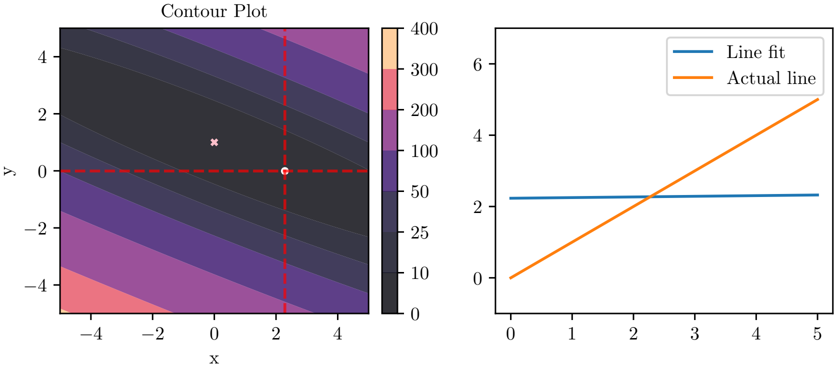
Gradient Descent : Example (Iteraion 16)



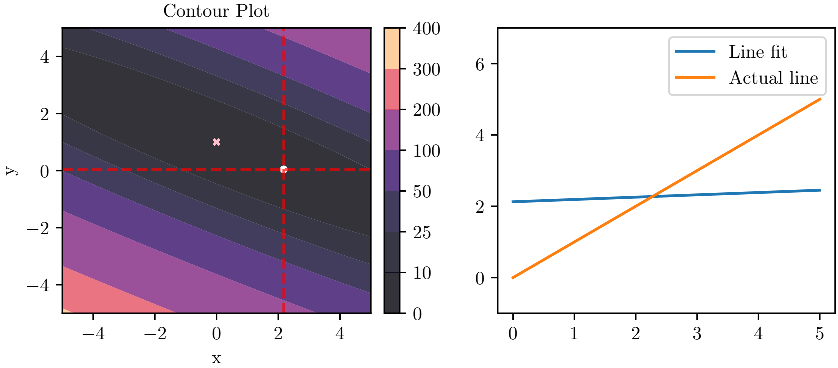
Gradient Descent : Example (Iteraion 18)



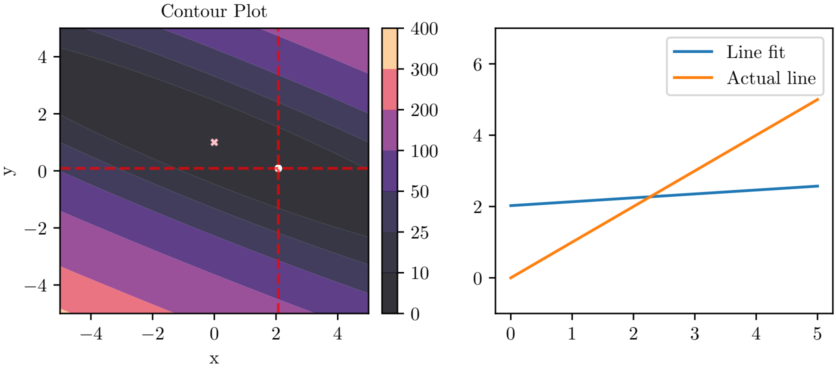
Gradient Descent : Example (Iteraion 20)



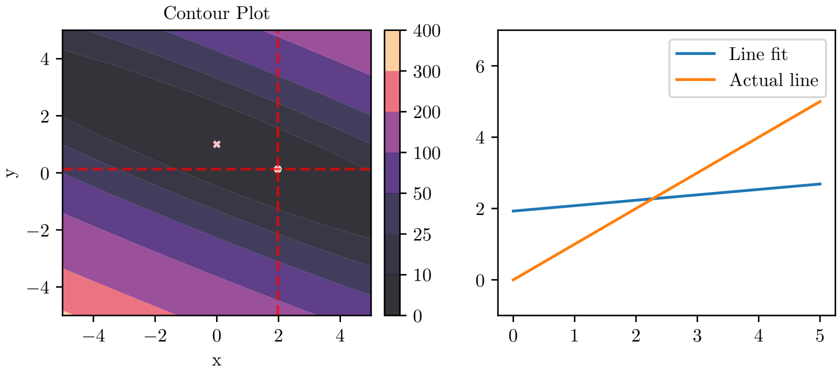
Gradient Descent : Example (Iteraion 22)



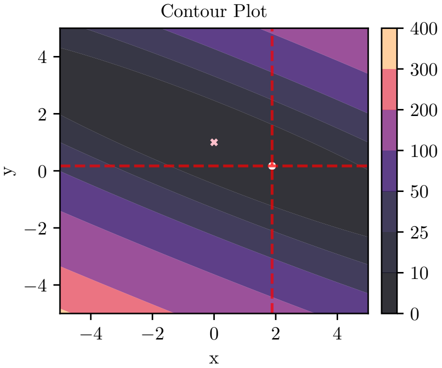
Gradient Descent : Example (Iteraion 24)

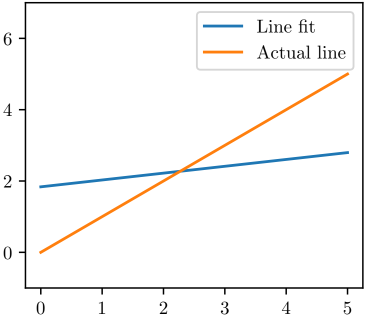


Gradient Descent : Example (Iteraion 26)

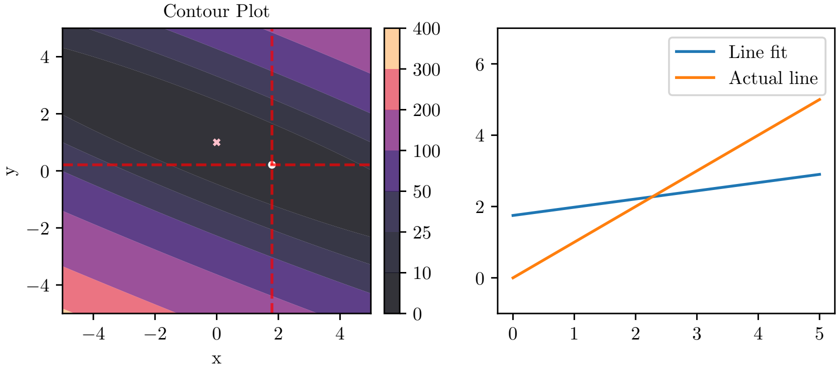


Gradient Descent : Example (Iteraion 28)

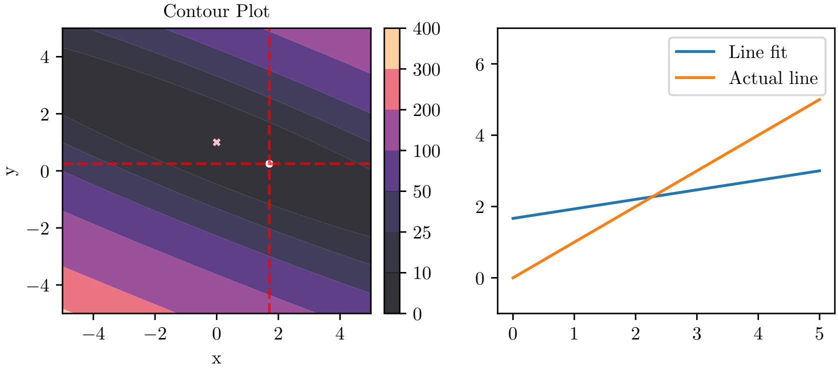




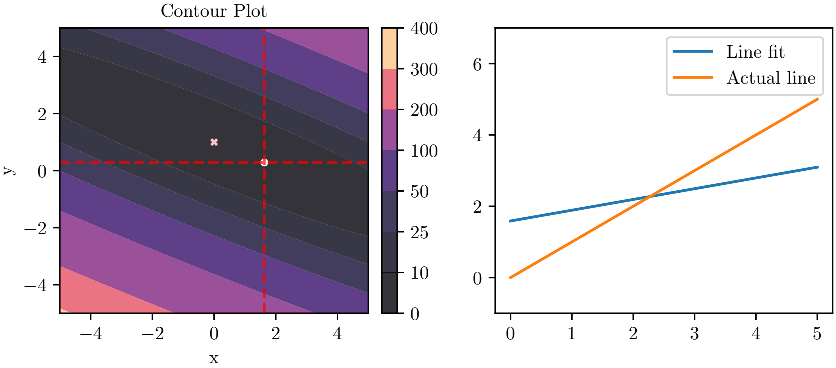
Gradient Descent : Example (Iteraion 30)



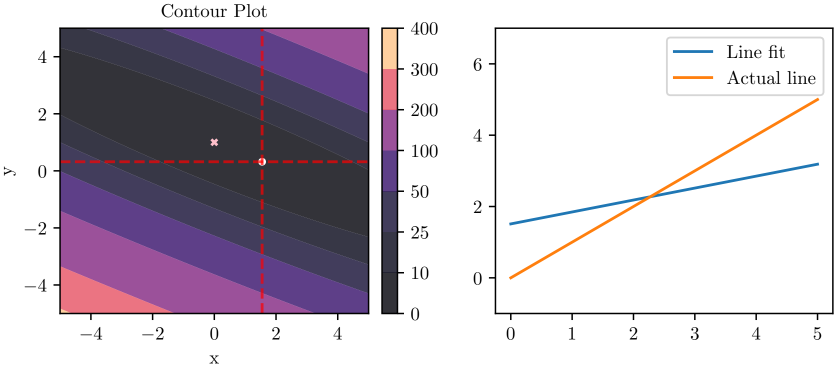
Gradient Descent : Example (Iteraion 32)



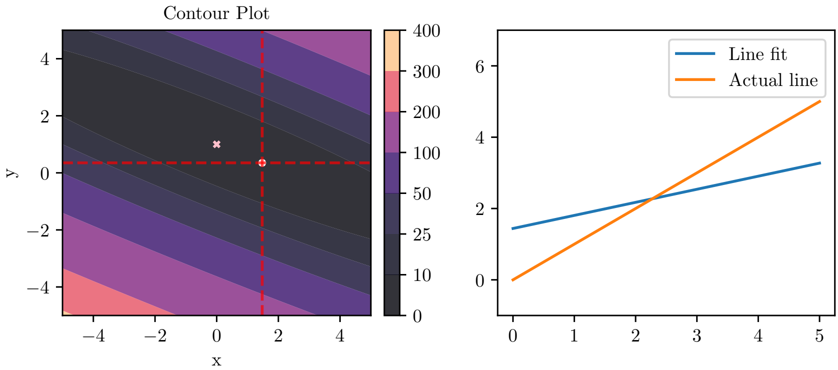
Gradient Descent : Example (Iteraion 34)



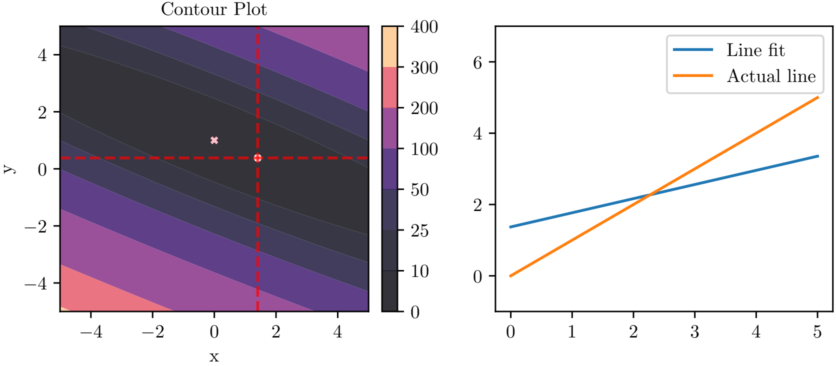
Gradient Descent : Example (Iteraion 36)



Gradient Descent : Example (Iteraion 38)



Gradient Descent : Example (Iteraion 40)



Iteration vs Epochs for gradient descent

- Iteration: Each time you update the parameters of the model

Iteration vs Epochs for gradient descent

- Iteration: Each time you update the parameters of the model
- Epoch: Each time you have seen all the set of examples

Gradient Descent (GD)

- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size n

Gradient Descent (GD)

- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size n
- Initialize $\boldsymbol{\theta}$

Gradient Descent (GD)

- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size n
- Initialize $\boldsymbol{\theta}$
- For epoch e in $[1, E]$

Gradient Descent (GD)

- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size *n*
- Initialize $\boldsymbol{\theta}$
- For epoch *e* in $[1, E]$
  - Predict $\hat{\mathbf{y}} = \text{pred}(\mathbf{X}, \boldsymbol{\theta})$

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  - Compute loss: $J(\boldsymbol{\theta}) = \text{loss}(\mathbf{y}, \hat{\mathbf{y}})$

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Stochastic Gradient Descent (SGD)

- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size *n*

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Stochastic Gradient Descent (SGD)

- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size n
- Initialize $\boldsymbol{\theta}$
- For epoch e in $[1, E]$
    - Shuffle $\mathcal{D}$

Stochastic Gradient Descent (SGD)

- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size *n*
- Initialize $\boldsymbol{\theta}$
- For epoch *e* in $[1, E]$
  - Shuffle $\mathcal{D}$
  - For *i* in $[1, n]$

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Mini-Batch Gradient Descent (MBGD)

- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size n

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- Dataset: $\mathcal{D} = \{(\mathbf{X}, \mathbf{y})\}$ of size n
- Initialize $\boldsymbol{\theta}$
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  - Batches $=$ make_batches$(\mathcal{D}, B)$

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Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data

Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost

Gradient Descent vs SGD

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- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

Gradient Descent vs SGD

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Gradient Descent vs SGD

Vanilla Gradient Descent

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Stochastic Gradient Descent

- In SGD, we update parameters after seeing each each point

Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost
- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

Stochastic Gradient Descent

- In SGD, we update parameters after seeing each each point
- Noisier curve for iteration vs cost

Gradient Descent vs SGD

Vanilla Gradient Descent

- in Vanilla (Batch) gradient descent: We update params after going through all the data
- Smooth curve for Iteration vs Cost
- For a single update, it needs to compute the gradient over all the samples. Hence takes more time

Stochastic Gradient Descent

- In SGD, we update parameters after seeing each each point
- Noisier curve for iteration vs cost
- For a single update, it computes the gradient over one example. Hence lesser time

Stochastic Gradient Descent : Example

Learn $y = \theta_0 + \theta_1 x$ on following dataset, using SGD where initially $(\theta_0, \theta_1) = (4, 0)$ and step-size, $\alpha = 0.1$, for 1 epoch (3 iterations).

x	**y**
2	2
3	3
1	1

Stochastic Gradient Descent : Example

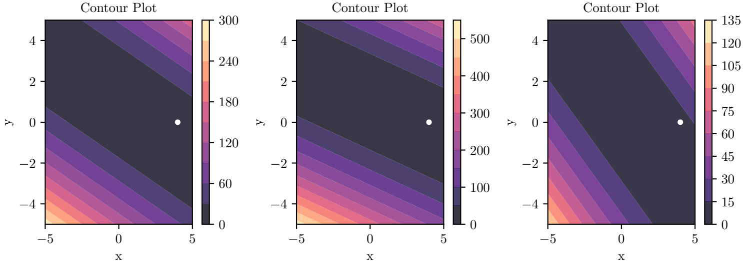
Our predictor, $\hat{y} = \theta_0 + \theta_1 x$

Error for i^{th} datapoint, $e_i = y_i - \hat{y}_i$
$\epsilon_1 = 2 - \theta_0 - 2\theta_1$
$\epsilon_2 = 3 - \theta_0 - 3\theta_1$
$\epsilon_3 = 1 - \theta_0 - \theta_1$

While using SGD, we compute the MSE using only 1 datapoint per iteration.
So MSE is ϵ_1^2 for iteration 1 and ϵ_2^2 for iteration 2.

Stochastic Gradient Descent : Example

Contour plot of the cost functions for the three datapoints



Stochastic Gradient Descent : Example

For Iteration *i*

$$\frac{\partial MSE}{\partial \theta_0} = 2\left(y_i - \theta_0 - \theta_1 x_i\right)(-1) = 2\epsilon_i(-1)$$

$$\frac{\partial MSE}{\partial \theta_1} = 2\left(y_i - \theta_0 - \theta_1 x_i\right)(-x_i) = 2\epsilon_i(-x_i)$$

Stochastic Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 4 - 0.1 \times 2 \times (2 - (4 + 0))\,(-1)$$

$$\theta_0 = 3.6$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 1

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 4 - 0.1 \times 2 \times (2 - (4 + 0))\,(-1)$$

$$\theta_0 = 3.6$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

$$\theta_1 = 0 - 0.1 \times 2 \times (2 - (4 + 0))\,(-2)$$

$$\theta_1 = -0.8$$

Stochastic Gradient Descent : Example

Iteration 2

$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$

$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$

Stochastic Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial \mathit{MSE}}{\partial \theta_0}$$

$$\theta_0 = 3.6 - 0.1 \times 2 \times (3 - (3.6 - 0.8 \times 3))\,(-1)$$

$$\theta_0 = 3.96$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial \mathit{MSE}}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 2

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

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$$\theta_0 = 3.96$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

$$\theta_0 = -0.8 - 0.1 \times 2 \times (3 - (3.6 - 0.8 \times 3))\,(-3)$$

$$\theta_1 = 0.28$$

Stochastic Gradient Descent : Example

Iteration 3

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

Stochastic Gradient Descent : Example

Iteration 3

$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$

$\theta_0 = 3.96 - 0.1 \times 2 \times (1 - (3.96 + 0.28 \times 1))\,(-1)$

$\theta_0 = 3.312$

$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$

Stochastic Gradient Descent : Example

Iteration 3

$$\theta_0 = \theta_0 - \alpha \frac{\partial MSE}{\partial \theta_0}$$

$$\theta_0 = 3.96 - 0.1 \times 2 \times (1 - (3.96 + 0.28 \times 1))\,(-1)$$

$$\theta_0 = 3.312$$

$$\theta_1 = \theta_1 - \alpha \frac{\partial MSE}{\partial \theta_1}$$

$$\theta_0 = 0.28 - 0.1 \times 2 \times (1 - (3.96 + 0.28 \times 1))\,(-1)$$

$$\theta_1 = -0.368$$

True Gradient

Based on Estimation Theory and Machine Learning by Florian Hartmann

- Let us say we have a dataset $\mathcal{D}$ containing input output pairs $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$

True Gradient

Based on Estimation Theory and Machine Learning by Florian Hartmann

- Let us say we have a dataset $\mathcal{D}$ containing input output pairs $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$
- We can define overall loss as:

$$L(\theta) = \frac{1}{N} \sum_{i=1}^{N} loss(f(x_i, \theta), y_i)$$

True Gradient

Based on Estimation Theory and Machine Learning by Florian Hartmann

- Let us say we have a dataset $\mathcal{D}$ containing input output pairs $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$
- We can define overall loss as:

$$L(\theta) = \frac{1}{N} \sum_{i=1}^{N} loss(f(x_i, \theta), y_i)$$

- loss can be any loss function such as squared loss, cross-entropy loss etc.

$$loss(f(x_i, \theta), y_i) = (f(x_i, \theta) - y_i)^2$$

True Gradient

- The true gradient of the loss function is given by:

$$\begin{aligned}\nabla L &= \nabla \frac{1}{n} \sum_{i=1}^{n} \operatorname{loss}\left(f\left(x_i\right), y_i\right) \\ &= \frac{1}{n} \sum_{i=1}^{n} \nabla \operatorname{loss}\left(f\left(x_i\right), y_i\right)\end{aligned}$$

True Gradient

- The true gradient of the loss function is given by:

$$\nabla L = \nabla \frac{1}{n} \sum_{i=1}^{n} \mathrm{loss}\left(f\left(x_i\right), y_i\right)$$
$$= \frac{1}{n} \sum_{i=1}^{n} \nabla \, \mathrm{loss}\left(f\left(x_i\right), y_i\right)$$

- The above is a consequence of linearity of the gradient operator.

Estimator for the true gradient

- In practice, we do not have access to the true gradient

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- We can only estimate the true gradient using a subset of the data
- For SGD, we use a single example to estimate the true gradient, for mini-batch gradient descent, we use a mini-batch of examples to estimate the true gradient
- Let us say we have a sample: (x, y)

Estimator for the true gradient

- In practice, we do not have access to the true gradient
- We can only estimate the true gradient using a subset of the data
- For SGD, we use a single example to estimate the true gradient, for mini-batch gradient descent, we use a mini-batch of examples to estimate the true gradient
- Let us say we have a sample: (x, y)
- The estimated gradient is given by:

$$\nabla \tilde{L} = \nabla \,\mathrm{loss}(f(x), y)$$

Bias of the estimator

- One measure for the quality of an estimator $\tilde{X}$ is its bias or how far off its estimate is on average from the true value X :
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$$\begin{aligned} \mathbb{E}[\nabla \tilde{L}] &= \sum_{i=1}^{n} \frac{1}{n} \nabla \operatorname{loss}\left(f\left(x_i\right), y_i\right) \\ &= \frac{1}{n} \nabla \sum_{i=1}^{n} \operatorname{loss}\left(f\left(x_i\right), y_i\right) \\ &= \nabla L \end{aligned}$$

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- Thus, the estimated gradient is an unbiased estimator of the true gradient

Normal Equation

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Normal Equation

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- What is the time complexity of solving the normal equation $\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$?

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- Scales cubic in the number of columns/features of $\mathbf{X}$

Gradient Descent

Start with random values of θ_0 and θ_1
Till convergence

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- $\theta_0 = \theta_0 - \alpha \frac{\partial}{\partial \theta_0} \left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\right)^\top \left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\right)$
  $\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} \left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\right)^\top \left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\right)$
  $\vdots$
  $\theta_d = \theta_d - \alpha \frac{\partial}{\partial \theta_d} \left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\right)^\top \left(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\right)$

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- $\boldsymbol{\theta} = \boldsymbol{\theta} - \alpha \frac{\partial}{\partial \boldsymbol{\theta}} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$

Gradient Descent

$$
\begin{aligned}
&\frac{\partial}{\partial \boldsymbol{\theta}}(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \\
&= \frac{\partial}{\partial \boldsymbol{\theta}}\left(\mathbf{y}^\top - \boldsymbol{\theta}^\top\mathbf{X}^\top\right)(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \\
&= \frac{\partial}{\partial \boldsymbol{\theta}}\left(\mathbf{y}^\top\mathbf{y} - \boldsymbol{\theta}^\top\mathbf{X}^\top\mathbf{y} - \mathbf{y}^\top\mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^\top\mathbf{X}^\top\mathbf{X}\boldsymbol{\theta}\right) \\
&= -2\mathbf{X}^\top\mathbf{y} + 2\mathbf{X}^\top\mathbf{X}\boldsymbol{\theta} \\
&= 2\mathbf{X}^\top(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})
\end{aligned}
$$

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We can write the vectorised update equation as follows, for each iteration
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All of the above need only be calculated once!

Gradient Descent

Gradient Descent

For each of the t iterations, we now need to first multiply $\alpha\mathbf{X}^\top\mathbf{X}$ with $\boldsymbol{\theta}$ which is matrix multiplication of a $d \times d$ matrix with a $d \times 1$, which is $\mathcal{O}(d^2)$

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What is overall computational complexity?
$\mathcal{O}(td^2)$ + $\mathcal{O}(d^2n) = \mathcal{O}((t+n)d^2)$

Gradient Descent (Alternative)

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If we do not rewrite the expression $\boldsymbol{\theta} = \boldsymbol{\theta} - \alpha \mathbf{X}^\top (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$
For each iteration, we have:

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$\mathcal{O}(ndt)$